

High-Order Summation-By-Parts Operators on Unstructured Grids

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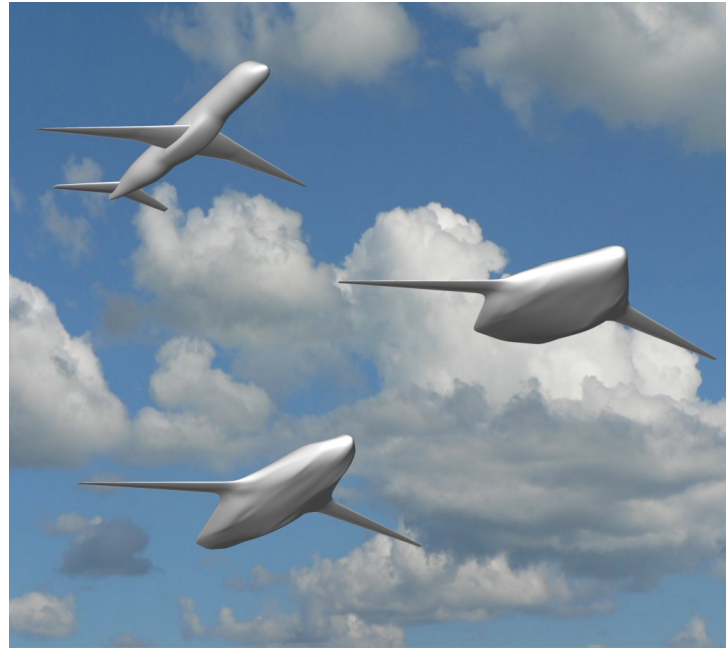
Advanced Modeling & Simulation (AMS) Seminar Series
NASA Ames Research Centre
10 August 2017

My Research Group

Research underway in the following areas:

- high-order discretization methods in time and space
 - summation-by-parts operators
 - implicit Runge-Kutta methods
- algorithms for aerodynamic shape optimization
 - two-level free-form deformation geometry control
 - integrated mesh movement method
 - enables substantial geometric flexibility (very large shape changes), analytical geometry representation
- application of aerodynamic shape optimization to unconventional energy-efficient aircraft configurations
- active flow control for drag reduction

Lifting Fuselage Configuration for Regional Class Aircraft



- shape found through RANS-based aerodynamic shape optimization
- narrower than classical hybrid wing-body
- centerbody carries about 30% of the lift (more than D8 for example)
- drag savings estimated at 6-10% relative to optimized conventional aircraft

Some recent papers that might be of interest

Reist, T.A., and Zingg, D.W., “High-Fidelity Aerodynamic Shape Optimization of a Lifting-Fuselage Concept for Regional Aircraft,” J. of Aircraft, Vol. 54, No. 3, 2017, pp. 1085-1097.

Reist, T.A., and Zingg, D.W., “Multi-Fidelity Optimization of Hybrid Wing-Body Aircraft with Stability and Control Requirements,” in preparation, 2017.

Rashad, R., and Zingg, D.W., “Aerodynamic Shape Optimization for Natural Laminar Flow Using a Discrete Adjoint Method,” AIAA J., Vol. 54, No. 11, 2016, pp. 3321-3337.

Gagnon, H., and Zingg, D.W., “Euler-Equation-Based Drag Minimization of Unconventional Aircraft Configurations,” J. of Aircraft, Vol. 53, No. 5, 2016, pp. 1361-1371.

Gagnon, H., and Zingg, D.W., “Aerodynamic Trade Study of a Box-Wing Aircraft Configuration,” J. of Aircraft, Vol. 53, No. 4, 2016, pp. 971-981.

Zhang, Z.J., Khosravi, S., and Zingg, D.W., “High-fidelity aerostructural optimization with integrated geometry parameterization and mesh movement,” Struct. Multidisc. Optim., Vol. 55, No. 4, 2017, pp. 1217-1235.

Boom, P.D., and Zingg, D.W., “Optimization of High-Order Diagonally Implicit Runge-Kutta Methods,” in preparation, 2017.

High-Order Methods

- huge potential efficiency benefits
- popular for large eddy and direct simulation of turbulent flows
- most production Reynolds-averaged Navier-Stokes solvers are second order
- singularities and discontinuities such as shocks are an issue
- robustness is an issue

Summation by Parts (SBP) Operators

- Operators constructed specifically to satisfy the SBP property
 - leads to provable time stability
 - usually used with simultaneous approximation terms (SATs) for weak imposition of boundary and interface conditions
- Other known operators satisfy the SBP property
 - some discontinuous Galerkin (DG) operators
 - some correction procedure by reconstruction (CPR) operators
 - some spectral collocation operators

“Discontinuous” Approaches

- Includes DG, CPR, and SBP-SAT approaches
 - SBP-SAT approach can also be implemented in a continuous manner
- High order achieved through interior degrees of freedom
- Have some nice properties that can be advantageous:
 - parallelization on modern computer architectures
 - reduced need for smooth meshes
- Potential disadvantage:
 - need for high order meshes

Classical (pre-2014) Summation by Parts Operators

$$\frac{\partial \mathcal{U}}{\partial x} \approx D\mathbf{u} = H^{-1}Q\mathbf{u}$$

where H is a (diagonal) symmetric positive-definite (SPD) matrix and

$$Q + Q^T = E = \begin{bmatrix} -1 & & & & \\ & 0 & & & \\ & & \ddots & & \\ & & & 0 & \\ & & & & 1 \end{bmatrix}$$

The norm matrix H defines an inner product, norm, and quadrature as

$$(\mathbf{u}, \mathbf{v})_H = \mathbf{u}^T H \mathbf{v} , \quad \|\mathbf{u}\|_H^2 = \mathbf{u}^T H \mathbf{u} , \quad \int_{x_L}^{x_R} \mathcal{U} dx \approx \mathbf{1}^T H \mathbf{u} , \quad \int_{x_L}^{x_R} \mathcal{U} \mathcal{V} dx \approx \mathbf{u}^T H \mathbf{v}$$

Integration by Parts

IBP (x derivative):

$$\int_{\Omega} \mathcal{V} \frac{\partial \mathcal{U}}{\partial x} d\Omega + \int_{\Omega} \mathcal{U} \frac{\partial \mathcal{V}}{\partial x} d\Omega = \oint_{\Gamma} \mathcal{V} \mathcal{U} n_x d\Gamma$$

Let $\mathcal{V} = \mathcal{U}$:

$$2 \int_{\Omega} \mathcal{U} \frac{\partial \mathcal{U}}{\partial x} d\Omega = \oint_{\Gamma} \mathcal{U}^2 n_x d\Gamma$$

Let $\mathcal{V} = 1$:

$$\int_{\Omega} \frac{\partial \mathcal{U}}{\partial x} d\Omega = \oint_{\Gamma} \mathcal{U} n_x d\Gamma$$

Summing over the three components of a vector gives the divergence theorem

SBP Discretely Mimics Integration by Parts

IBP (x derivative):

$$\int_{\Omega} \mathcal{V} \frac{\partial \mathcal{U}}{\partial x} d\Omega + \int_{\Omega} \mathcal{U} \frac{\partial \mathcal{V}}{\partial x} d\Omega = \oint_{\Gamma} \mathcal{V} \mathcal{U} n_x d\Gamma$$

IBP (one dimension):

$$\int_{x_L}^{x_R} \mathcal{V} \frac{\partial \mathcal{U}}{\partial x} dx + \int_{x_L}^{x_R} \mathcal{U} \frac{\partial \mathcal{V}}{\partial x} dx = \mathcal{V} \mathcal{U} \Big|_{x_L}^{x_R}$$

SBP:

$$\mathbf{v}^T H D \mathbf{u} + \mathbf{u}^T H D \mathbf{v} = \mathbf{v}^T E \mathbf{u} = v_R u_R - v_L u_L$$

Setting $\mathbf{v} = \mathbf{u}$ gives

$$2\mathbf{u}^T H D \mathbf{u} = \mathbf{u}^T E \mathbf{u} = u_R^2 - u_L^2$$

Observe that this makes the role of E clear:

$$\mathbf{v}^T E \mathbf{u} \approx \oint_{\Gamma} \mathcal{V} \mathcal{U} n_x d\Gamma$$

Linear Convection Equation: Well Posedness

Linear convection equation:

$$\frac{\partial \mathcal{U}}{\partial t} = -\frac{\partial \mathcal{U}}{\partial x}, \quad x_L \leq x \leq x_R, \quad \mathcal{U}(x_L, t) = \mathcal{U}_L(t)$$

Multiply by $2\mathcal{U}$ and integrate over the domain:

$$\int_{x_L}^{x_R} \frac{\partial \mathcal{U}^2}{\partial t} dx = - \int_{x_L}^{x_R} \frac{\partial \mathcal{U}^2}{\partial x} dx$$

$$\frac{d}{dt} \int_{x_L}^{x_R} \mathcal{U}^2 dx = -(\mathcal{U}_R^2 - \mathcal{U}_L^2) \leq 0 \quad \text{if } \mathcal{U}_L = 0$$

Semi-Discrete Form

$$\frac{d\mathbf{u}}{dt} = -D\mathbf{u} = -H^{-1}Q\mathbf{u}$$

Multiply by $2\mathbf{u}^T H$:

$$\begin{aligned} 2\mathbf{u}^T H \frac{d\mathbf{u}}{dt} &= -2\mathbf{u}^T H D \mathbf{u} = -2\mathbf{u}^T H H^{-1} Q \mathbf{u} = -2\mathbf{u}^T Q \mathbf{u} \\ \frac{d\|\mathbf{u}\|_H^2}{dt} &= -2\mathbf{u}^T \left(\frac{Q + Q^T}{2} \right) \mathbf{u} = -\mathbf{u}^T E \mathbf{u} = -(u_n^2 - u_1^2) \end{aligned}$$

Mimics continuous result because

$$Q + Q^T = E = \begin{bmatrix} -1 & & & & \\ & 0 & & & \\ & & \ddots & & \\ & & & 0 & \\ & & & & 1 \end{bmatrix}$$

Classical finite-difference SBP operator ($p = 1$)

$$D = H^{-1}Q$$

Gives a first-order (p) approximation to the first derivative (at the boundary nodes) and second-order ($2p$) in the interior, which will produce a second-order ($p + 1$) solution to the linear convection equation (for diagonal H)

$$H = \Delta x \begin{bmatrix} 1/2 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & & 1/2 \end{bmatrix} \quad (\text{composite trapezoidal rule})$$

$$Q = \begin{bmatrix} -1/2 & 1/2 & & & \\ -1/2 & 0 & 1/2 & & \\ & \ddots & \ddots & \ddots & \\ & & -1/2 & 0 & 1/2 \\ & & & -1/2 & 1/2 \end{bmatrix}$$

N.B. Functional superconvergence for dual consistent formulations

A classical finite-difference SBP operator ($p = 2$)

Gives a second-order (p) approximation to the first derivative (at the near-boundary nodes) and fourth-order ($2p$) in the interior, which will produce a third-order ($p + 1$) solution to the linear convection equation (for diagonal H)

$$D = H^{-1}Q$$

$$H = \Delta x \begin{bmatrix} 17/48 & & & & & \\ & 59/48 & & & & \\ & & 43/48 & & & \\ & & & 49/48 & & \\ & & & & 1 & \\ & & & & & \ddots \end{bmatrix} \quad (\text{Gregory rule})$$

$$Q = \begin{bmatrix} -1/2 & 59/96 & -1/12 & -1/32 & & & \\ -59/96 & 0 & 59/96 & 0 & & & \\ 1/12 & -59/96 & 0 & 59/96 & -1/12 & & \\ 1/32 & 0 & -59/96 & 0 & 8/12 & -1/12 & \\ 0 & 0 & 1/12 & -8/12 & 0 & 8/12 & -1/12 \\ & & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}$$

Boundary and Interface Conditions: Simultaneous Approximation Terms (SATs)

- weak imposition of boundary and interface conditions
 - penalty methods
- discontinuous solutions
- similar to discontinuous Galerkin finite-element methods

Stability

$$\frac{d\mathbf{u}}{dt} = -H^{-1}Q\mathbf{u} - H^{-1}(u_1 - \mathcal{U}_L)\mathbf{e}_1$$

where $\mathbf{e}_1 = [1, 0, \dots, 0]^T$

Gives, for $\mathcal{U}_L = 0$:

$$\frac{d\|\mathbf{u}\|_H^2}{dt} = -2\mathbf{u}^T Q\mathbf{u} - 2\mathbf{u}^T(u_1)\mathbf{e}_1 = -(u_n^2 - u_1^2) - u_1^2 = -(u_n^2 + u_1^2) \leq 0$$

Conservation at Interfaces: Two Neighbouring Blocks

Conservation

$$\begin{aligned}\frac{d\mathbf{u}_L}{dt} &= -H_L^{-1}Q_L\mathbf{u}_L - H_L^{-1}(u_1^L - \mathcal{U}_L)\mathbf{e}_1 \\ \frac{d\mathbf{u}_R}{dt} &= -H_R^{-1}Q_R\mathbf{u}_R - H_R^{-1}(u_1^R - u_{n_L}^L)\mathbf{e}_1\end{aligned}$$

Gives:

$$\begin{aligned}\mathbf{1}^T H_L \frac{d\mathbf{u}_L}{dt} &= -(u_{n_L}^L - \mathcal{U}_L) \\ \mathbf{1}^T H_R \frac{d\mathbf{u}_R}{dt} &= -(u_{n_R}^R - u_{n_L}^L)\end{aligned}$$

$$\mathbf{1}^T H_L \frac{d\mathbf{u}_L}{dt} + \mathbf{1}^T H_R \frac{d\mathbf{u}_R}{dt} = -(u_{n_R}^R - \mathcal{U}_L)$$

Symmetric SATs are also possible

Generalized Summation by Parts (GSBP) Property

- Introduces the following three generalizations:
 - nonuniform nodal distributions
 - no repeating interior operator
 - operators without nodes on one or both boundaries
- With these generalizations it can be shown that some existing operators satisfy the GSBP property
- Enables the construction of novel operators (because no basis functions are needed explicitly)
- No longer restricted to Gregory quadrature rules

Generalized Summation by Parts Operators: Definition

An operator D is an approximation to the first derivative of degree p with the SBP property if the accuracy condition is met, H is an SPD matrix, and

$$Q + Q^T = E$$

where $(\mathbf{x}^i)^T E \mathbf{x}^j = (x_R)^{i+j} - (x_L)^{i+j}$, $i, j \in [0, r]$, $r \geq p$

E can be constructed as

$$E = \mathbf{t}_R \mathbf{t}_R^T - \mathbf{t}_L \mathbf{t}_L^T$$

where \mathbf{t}_L and \mathbf{t}_R satisfy

$$\mathbf{t}_L^T \mathbf{x}^j = x_L^j, \quad \mathbf{t}_R^T \mathbf{x}^j = x_R^j, \quad j \in [0, r]$$

This means that $\mathbf{t}_L^T \mathbf{u} \approx \mathcal{U}_L$, $\mathbf{t}_R^T \mathbf{u} \approx \mathcal{U}_R$ and we get

$$\mathbf{v}^T E \mathbf{u} \approx \mathcal{V}_R \mathcal{U}_R - \mathcal{V}_L \mathcal{U}_L \quad \text{for SBP}$$

$$\text{and hence } \mathbf{u}^T E \mathbf{u} \approx \mathcal{U}_R^2 - \mathcal{U}_L^2 \quad \text{for stability (with SAT)}$$

Generalized SBP example: nonuniform nodal distribution

Hybrid Gauss-trapezoidal-Lobatto quadrature nodal distribution given for 9 nodes by $(x \in [0, 1])$:

$$x = \frac{1}{8} \left[0 \quad \frac{12}{13} \quad 2 \quad 3 \quad 4 \quad 5 \quad 6 \quad \left(8 - \frac{12}{13}\right) \quad 8 \right]^T$$

$$D = 8 \begin{bmatrix} -\frac{864}{553} & \frac{408811}{209034} & -\frac{2901}{7742} & -\frac{278}{14931} & & & & & \\ -\frac{41}{78} & 0 & \frac{15}{26} & -\frac{2}{39} & & & & & \\ \frac{967}{7932} & -\frac{49855}{71388} & 0 & \frac{11800}{17847} & -\frac{56}{661} & & & & \\ \frac{139}{23460} & \frac{9971}{164220} & -\frac{1770}{2737} & 0 & \frac{1296}{1955} & -\frac{162}{1955} & & & \\ & & \frac{1}{12} & -\frac{2}{3} & 0 & \frac{2}{3} & -\frac{1}{12} & & \\ & & & \frac{162}{1955} & -\frac{1296}{1955} & 0 & \frac{1770}{2737} & -\frac{9971}{164220} & -\frac{139}{23460} \\ & & & & \frac{56}{661} & -\frac{11800}{17847} & 0 & \frac{49855}{71388} & -\frac{967}{7932} \\ & & & & & \frac{2}{39} & -\frac{15}{26} & 0 & \frac{41}{78} \\ & & & & & \frac{278}{14931} & \frac{2901}{7742} & -\frac{408811}{209034} & \frac{864}{553} \end{bmatrix}$$

Includes a standard interior operator that can be repeated

Second generalized SBP example: nonuniform nodal distribution with no repeating interior operator

Diagonal-norm operator on Chebyshev-Gauss-Lobatto quadrature nodal distribution given for 5 nodes by ($x \in [0, 1]$):

$$x = \frac{1}{2} \begin{bmatrix} -1 & -\frac{1}{2}\sqrt{2} & 0 & \frac{1}{2}\sqrt{2} & 1 \end{bmatrix}^T + \left(\frac{1}{2}\right) \mathbf{1}$$

where $\mathbf{1}$ is a vector of ones

$$D = 2 \begin{bmatrix} -\frac{15}{2} & 8 + 2\sqrt{2} & -6 & 8 - 2\sqrt{2} & -\frac{5}{2} \\ -1 - \frac{1}{4}\sqrt{2} & 0 & \frac{3}{2}\sqrt{2} & -\sqrt{2} & 1 - \frac{1}{4}\sqrt{2} \\ \frac{1}{2} & -\sqrt{2} & 0 & \sqrt{2} & -\frac{1}{2} \\ -1 + \frac{1}{4}\sqrt{2} & \sqrt{2} & -\frac{3}{2}\sqrt{2} & 0 & 1 + \frac{1}{4}\sqrt{2} \\ \frac{5}{2} & -8 + 2\sqrt{2} & 6 & -8 - 2\sqrt{2} & \frac{15}{2} \end{bmatrix}$$

Third generalized SBP example: nonuniform nodal distribution with no repeating interior operator and no boundary nodes

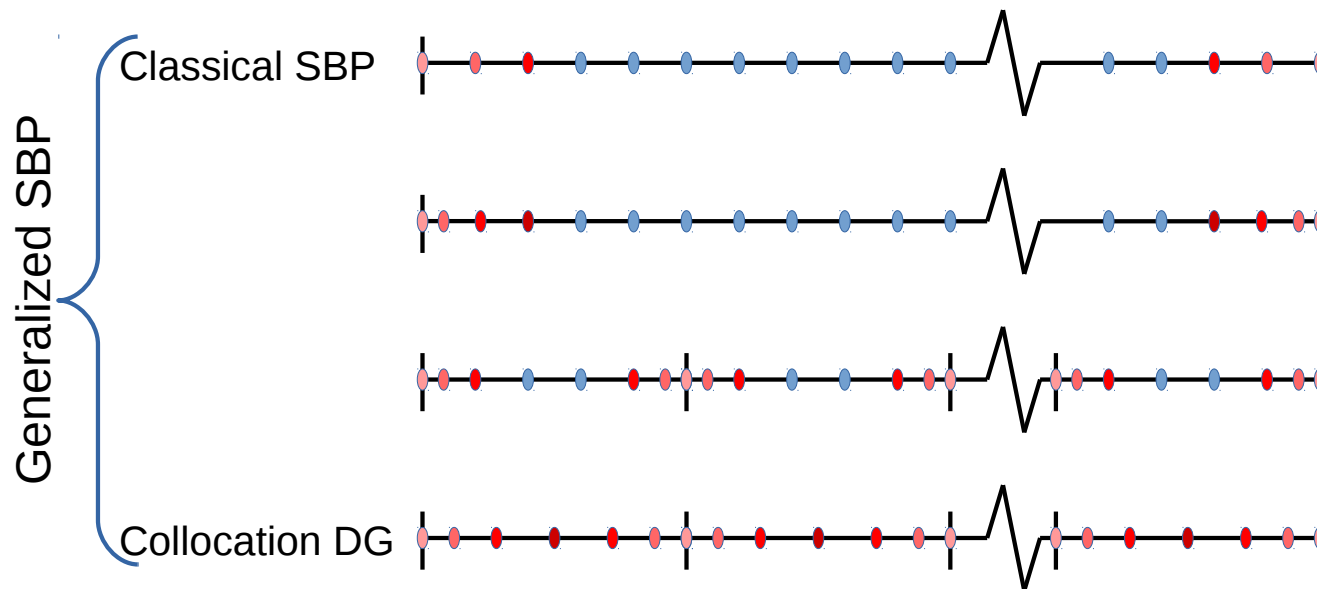
Diagonal-norm operator on Legendre-Gauss quadrature nodal distribution given for 3 nodes by $(x \in [0, 1])$:

$$\mathbf{x} = \frac{1}{2} \left[-\frac{\sqrt{15}}{5}, 0, \frac{\sqrt{15}}{5} \right]^T + \left(\frac{1}{2} \right) \mathbf{1}$$

where $\mathbf{1}$ is a vector of ones

$$D = 2 \begin{bmatrix} -\frac{1}{2}\sqrt{15} & \frac{2}{3}\sqrt{15} & -\frac{1}{6}\sqrt{15} \\ -\frac{1}{6}\sqrt{15} & 0 & \frac{1}{6}\sqrt{15} \\ \frac{1}{6}\sqrt{15} & -\frac{2}{3}\sqrt{15} & \frac{1}{2}\sqrt{15} \end{bmatrix}$$

Generalized SBP Operators



- classical SBP operators are applied in the traditional finite-difference manner
 - uniform meshes in computational space, repeating interior operator
- generalized SBP operators can be applied in an element-type manner, can have repeating interior operator or not, can have uniform or nonuniform nodal distribution

Element-type Finite-Difference Methods

	basis functions	elements	Taylor series	repeating interior operator
finite-difference method	✗	✗	✓	✓
finite-element method	✓	✓	✗	✗
element-type finite-difference method	✗	optional	✓	optional

Multidimensional GSBP Operators: some notation

In two dimensions:

$$\begin{aligned} S &= (x_i, y_i)_{i=1}^n \\ \mathbf{u} &= [\mathcal{U}(x_1, y_1), \dots, \mathcal{U}(x_n, y_n)]^T \end{aligned}$$

Monomials of total degree p (size in 2D: $n_p^* = (p+1)(p+2)/2$):

$$\begin{aligned} \mathcal{P}_k(x, y) &\equiv x^i y^{j-i}, \quad k = j(j+1)/2 + i + 1 \quad \forall j \in [0, 1, \dots, p], \quad i \in [0, 1, \dots, j] \\ \mathbf{p}_k &\equiv [\mathcal{P}_k(x_1, y_1), \dots, \mathcal{P}_k(x_n, y_n)]^T \\ \mathbf{p}'_k &\equiv \left[\frac{\partial \mathcal{P}_k}{\partial x}(x_1, y_1), \dots, \frac{\partial \mathcal{P}_k}{\partial x}(x_n, y_n) \right]^T \end{aligned}$$

Two-Dimensional GSBP Operator: definition

1. accuracy to degree p :

$$D_x \mathbf{p}_k = \mathbf{p}'_k \quad \forall k \in [1, 2, \dots, n_p^*]$$

2. $D_x = H^{-1}Q_x$ where H is symmetric positive definite (focus on diagonal H)

3. to mimic IBP:

$$Q_x + Q_x^T = E_x, \text{ which satisfies } \mathbf{p}_k^T E_x \mathbf{p}_m = \oint_{\Gamma} \mathcal{P}_k \mathcal{P}_m n_x d\Gamma \quad \forall k, m \in [1, 2, \dots, n_{\tau}^*]$$

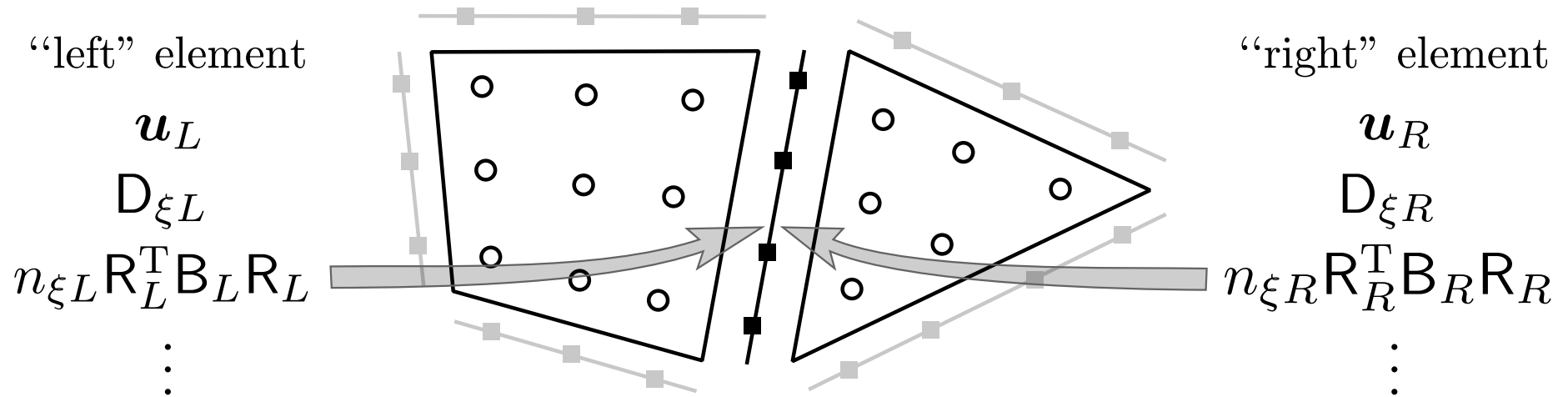
where $\tau \geq p$

Mimics integration by parts as in the 1D case:

$$\int_{\Omega} \mathcal{V} \frac{\partial \mathcal{U}}{\partial x} d\Omega + \int_{\Omega} \mathcal{U} \frac{\partial \mathcal{V}}{\partial x} d\Omega = \oint_{\Gamma} \mathcal{V} \mathcal{U} n_x d\Gamma \Leftrightarrow \mathbf{v}^T H D_x \mathbf{u} + \mathbf{u}^T H D_x \mathbf{v} = \mathbf{v}^T E_x \mathbf{u}$$

(exact for $\mathbf{p}_k, \mathbf{p}_m$ where $k, m \leq n_p^*$)

Construction of E_ξ and Application of SATs

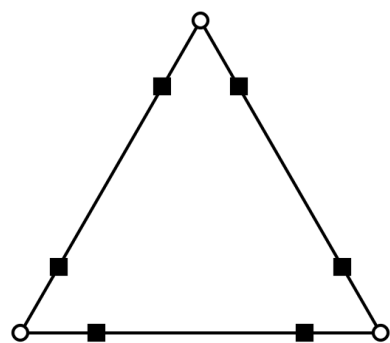


- open circles are the volume nodes at which the solution is stored
- black squares are the cubature nodes for the face used in decomposition of E and application of SATs
- $B_{L/R}$ hold the cubature weights
- $R_{L/R}$ are interpolation/extrapolation operators from the volume nodes to the face cubature nodes
- SATs are applied in a pointwise manner at the face cubature nodes

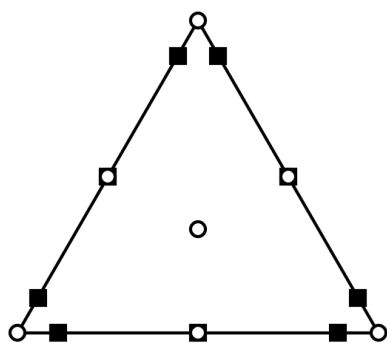
Construction of Operators

1. Choose or construct a symmetric cubature rule of total degree $2p - 1$ on a nodal distribution with at least n_p^* nodes – gives diagonal H
2. Choose or construct a cubature rule and nodal distribution for the faces (e.g. Legendre-Gauss with $p + 1$ nodes) – gives B
3. Construct the interpolation/extrapolation operators R from volume nodes to face nodes
4. Construct matrices E_ξ and E_η
5. Determine matrices Q_ξ and Q_η from the accuracy conditions

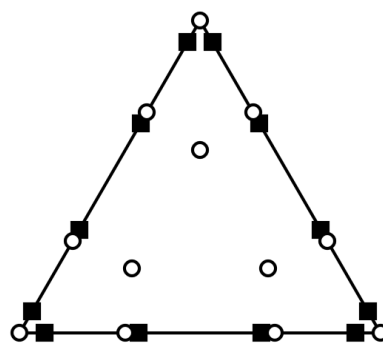
Two Example Families of Operators



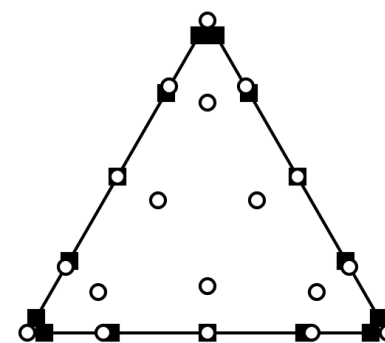
$p = 1$



$p = 2$

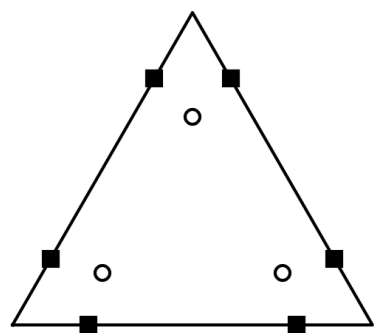


$p = 3$

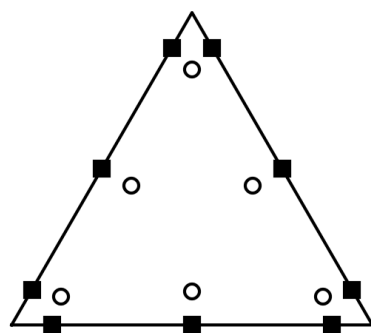


$p = 4$

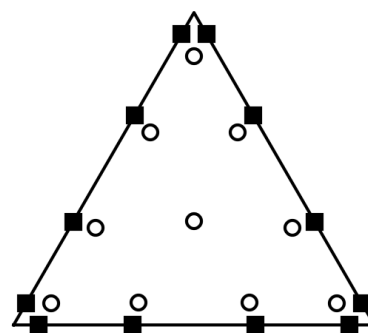
SBP- Γ family of operators with $p + 1$ nodes on each face



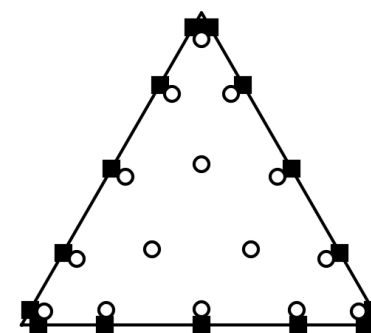
$p = 1$



$p = 2$



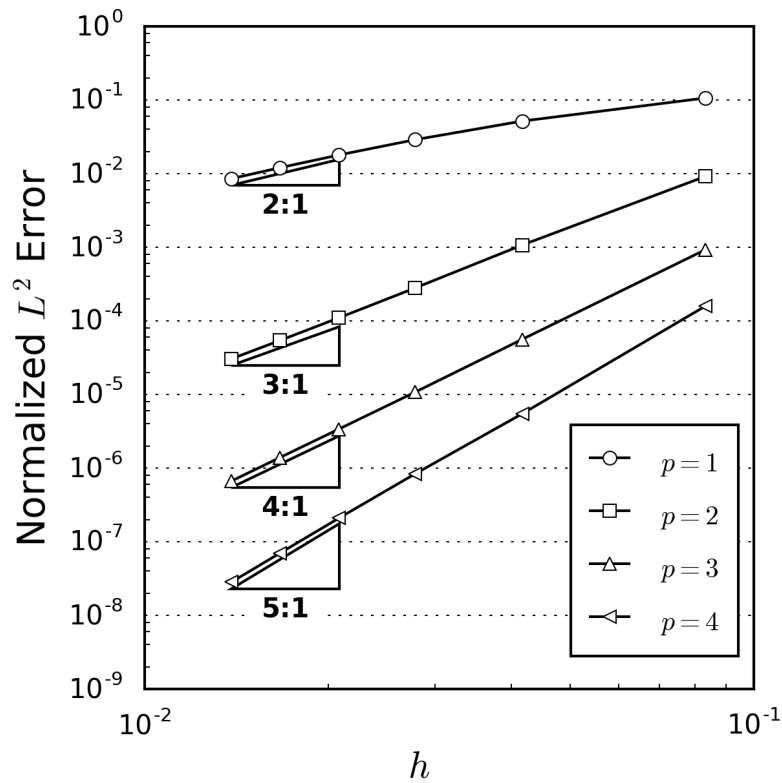
$p = 3$



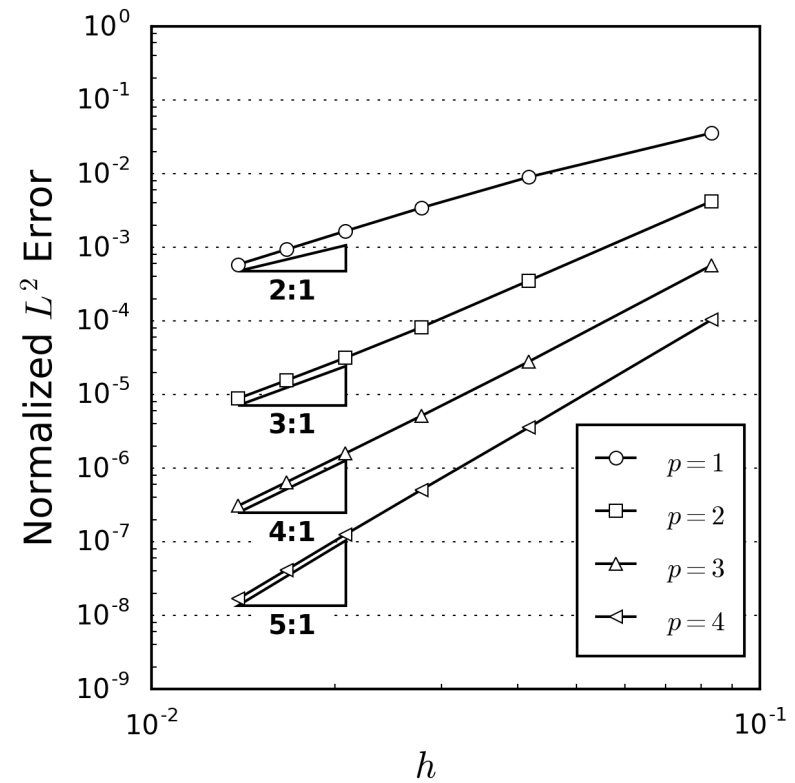
$p = 4$

SBP- Ω family of operators with nodes only in the interior of the element

Accuracy (2D linear convection on curvilinear mesh)



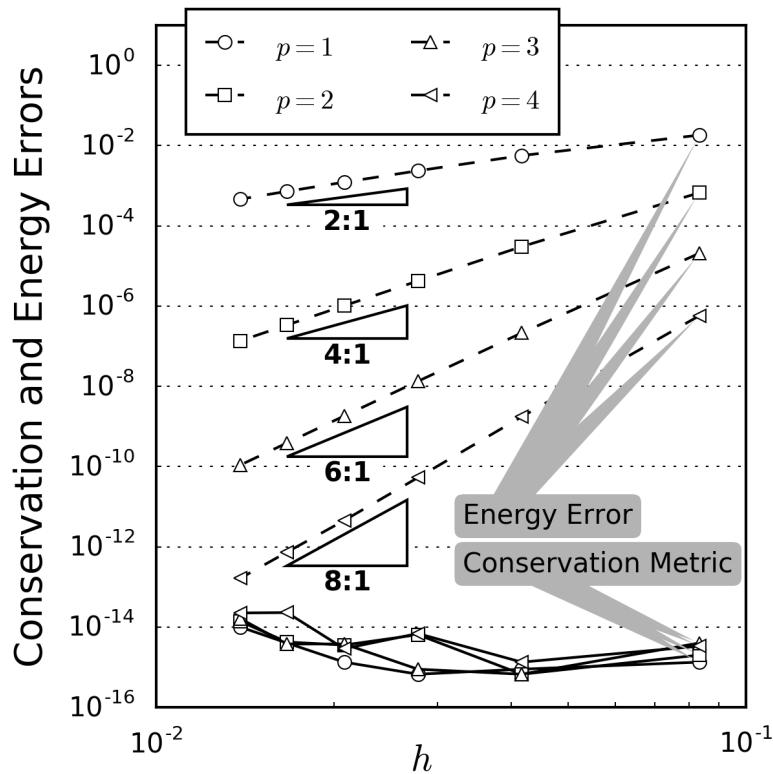
SBP- Γ family



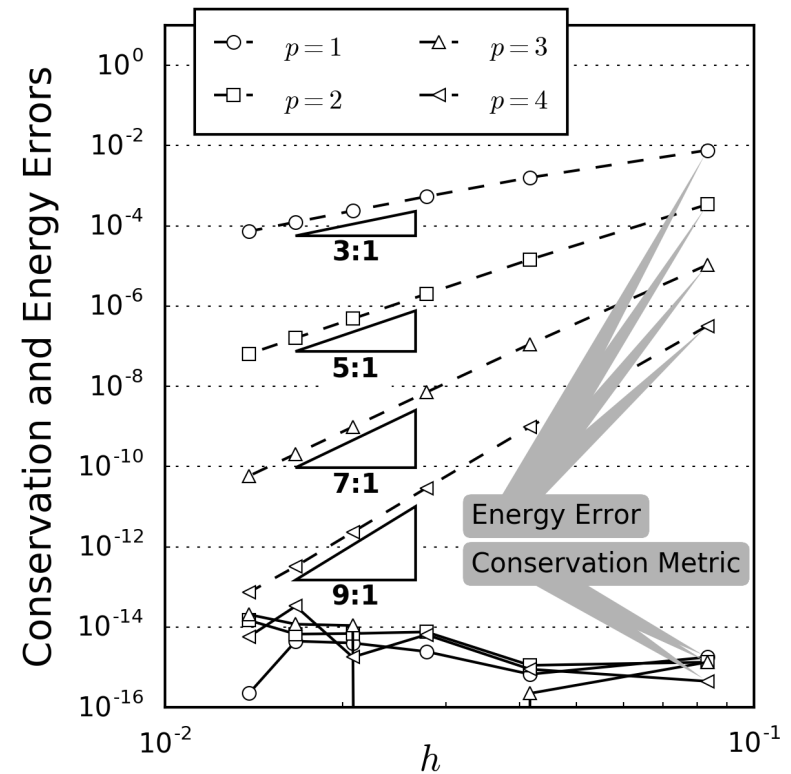
SBP- Ω family

- periodic boundary conditions, divergence-free velocity field
- convergence rates of $O(h^{p+1})$ typically achieved
- consistent trends on highly nonsmooth meshes

Conservation and Stability



SBP- Γ family



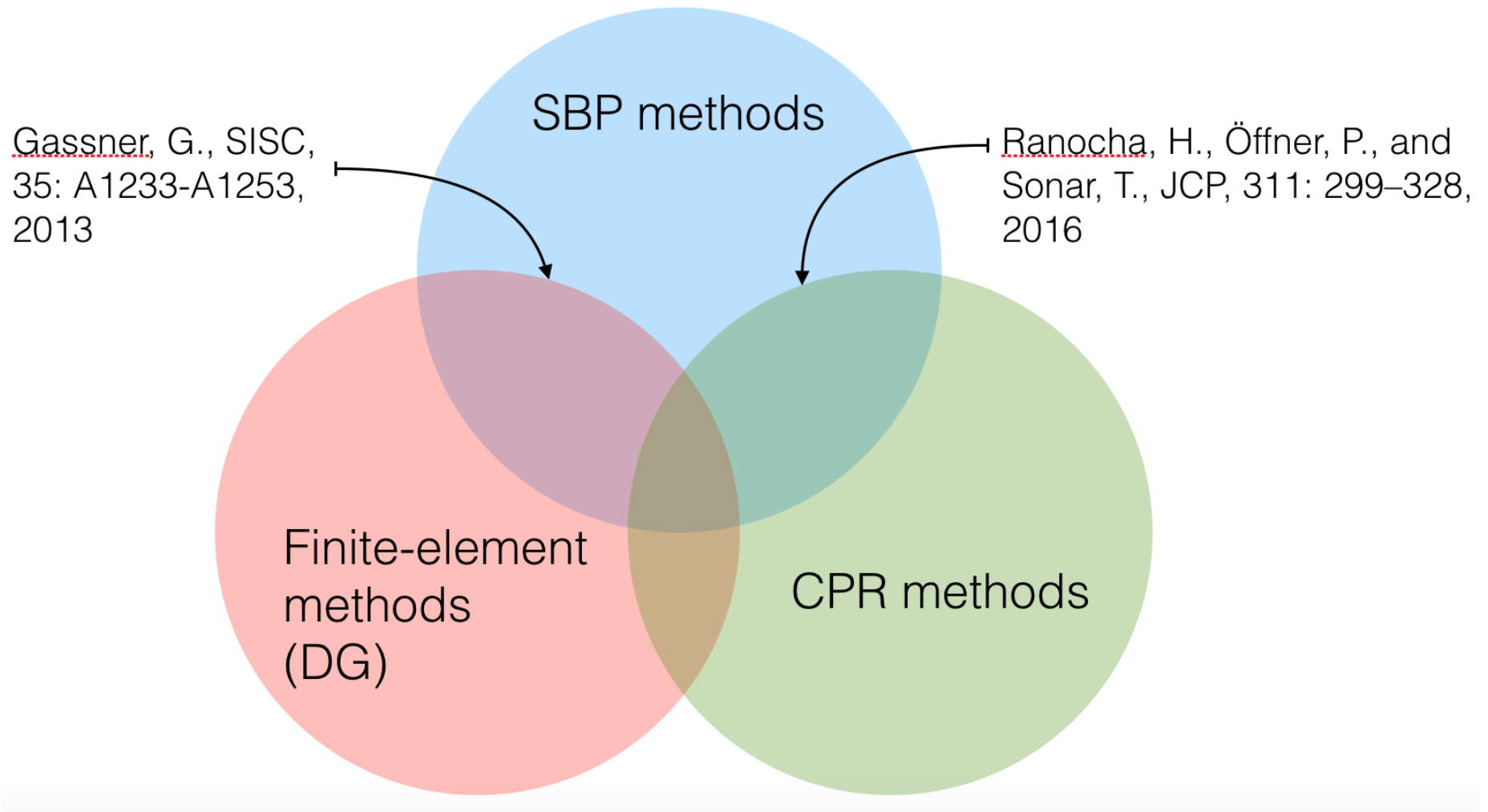
SBP- Ω family

- conservative to machine precision ($\mathbf{1}^T H_g \mathbf{u}_0 - \mathbf{1}^T H_g \mathbf{u}$)
- energy stable (skew-symmetric form solved with upwind SATs)
- superlinear convergence of energy reduction ($\mathbf{u}_0^T H_g \mathbf{u}_0 - \mathbf{u}^T H_g \mathbf{u}$)

Conclusions

- The multi-dimensional summation-by-parts property is a powerful means of developing stable (and hence robust) high-order operators for unstructured grids
 - concept can be exploited in discontinuous Galerkin and flux reconstruction methods as well as in SBP operators
- Multi-dimensional summation-by-parts operators represent a potentially powerful option for high-order methods
 - very general as a result of the absence of explicit basis functions in their derivation
 - increased flexibility and generality can be exploited in various ways
- Recent extension to multi-dimensions opens up new opportunities for unstructured grids
 - much work remains to be done to unlock the potential of SBP operators!

Relationship Between SBP, DG, and CPR?



- are there methods that are advantageous in certain respects or contexts that lie only within the SBP circle?

Further Reading

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